

Better estimation of small Sobol' sensitivity indices

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Abstract

A new method for estimating Sobol' indices is proposed. The new method makes use of 3 independent input vectors rather than the usual 2. It attains much greater accuracy on problems where the target Sobol' index is small, even outperforming some oracles which adjust using the true but unknown mean of the function. When the target Sobol' index is quite large, the oracles do better than the new method.

1 Introduction

Let f be a deterministic function on $[0, 1]^d$ for $d \geq 1$. Sobol' sensitivity indices, derived from a functional ANOVA, are used to measure the importance of subsets of input variables. There are two main types of index, but one of them is especially hard to estimate in cases where that index is small.

The problematic index can be represented as a covariance between outcomes of f evaluated at two random input points, that share some but not all of their components. A natural estimator then is a sample covariance based on pairs of random d -vectors of this type. Sobol' and Myshetskaya (2007) report a numerical experiment where enormous efficiency differences obtain depending on how one estimates that covariance. The best gains arise from applying some centering strategies to those pairs of function evaluations.

This article introduces a new estimator for the Sobol' index, based on three input vectors, not two. The new estimator makes perhaps surprising use of randomly generated centers. The random centering adds to the cost of every simulation run and might be thought to add noise. But in many examples that noise must be strongly negatively correlated with the quantity it adjusts because (in those examples) the random centering greatly increases efficiency. The new estimate is not always most efficient. In particular when the index to be estimated is large the new estimate is seen to perform worse than some oracles that one could approximate numerically.

The motivation behind Sobol' indices, is well explained in the text by Saltelli et al. (2008). These indices have been applied to problems in industry, science and

public health. For a recent mathematical account of Sobol' indices, see Owen (2012).

The outline of this article is as follows. Section 2 introduces Sobol' indices and our notation. Section 3 presents the original estimator of the Sobol' indices and the four improved estimators we consider here. Section 4 considers some numerical examples. For small Sobol' indices, the newly proposed estimator is best, beating two oracles. For very large indices, the best performance comes from an oracle that uses the true function mean twice. Section 5 presents some theoretical support for the new estimator. It generalizes the estimator to a wider class of methods and shows that the proposed estimator minimizes a proxy for the variance, when one considers functions of product form.

2 Background

For $d \geq 1$, let $f \in L^2[0, 1]^d$. Then f can be written in an ANOVA decomposition as a sum of a constant $\mu = \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x}$ and $2^d - 1$ mutually orthogonal ANOVA effects, one for each nonempty subset of $\mathcal{D} = \{1, 2, \dots, d\}$. The effect for non-empty subset $u \subseteq \mathcal{D}$ has variance σ_u^2 , while $\sigma_\emptyset^2 = 0$. A larger σ_u^2 means a more important interaction among those variables, but Sobol' indices account for the fact that the importance of a set of variables also depends on other interactions in which they participate.

The two most important Sobol' indices are

$$\mathcal{I}_u^2 = \sum_{v \subseteq u} \sigma_v^2, \quad \text{and} \quad (1)$$

$$\bar{\tau}_u^2 = \sum_{v \cap u \neq \emptyset} \sigma_v^2. \quad (2)$$

These satisfy $0 \leq \mathcal{I}_u^2 \leq \bar{\tau}_u^2 \leq \sigma^2$ and $\mathcal{I}_u^2 = \sigma^2 - \bar{\tau}_{-u}^2$, where σ^2 is the variance $\int (f(\mathbf{x}) - \mu)^2 d\mathbf{x}$. We use $-u$ or u^c depending on typographical readability, to denote the complement of u in \mathcal{D} . These indices provide two measures of the importance of the variables in subset u . The larger measure includes interactions between variables in u and variables in its complement, while the smaller measure excludes those interactions.

If we unite the part of $\mathbf{x} \in [0, 1]^d$ corresponding to indices in the set u with the part of another point $\mathbf{y} \in [0, 1]^d$ for indices in $-u$, then the resulting point is denoted $\mathbf{x}_u : \mathbf{y}_{-u}$. Most estimation strategies for Sobol' indices are based on the identities

$$\mathcal{I}_u^2 = \mu^2 + \int f(\mathbf{x}) f(\mathbf{x}_u : \mathbf{y}_{-u}) d\mathbf{x} d\mathbf{y}, \quad \text{and} \quad (3)$$

$$\bar{\tau}_u^2 = \frac{1}{2} \int (f(\mathbf{x}) - f(\mathbf{x}_u : \mathbf{y}_{-u}))^2 d\mathbf{x} d\mathbf{y}, \quad (4)$$

with integrals taken over \mathbf{x} and $\mathbf{y} \in [0, 1]^d$.

When τ_u^2 is small, then (4) leads to a very effective Monte Carlo strategy based on

$$\hat{\tau}_u^2 = \frac{1}{2n} \sum_{i=1}^n (f(\mathbf{x}_i) - f(\mathbf{x}_{i,u}:\mathbf{y}_{i,-u}))^2$$

for $(\mathbf{x}_i, \mathbf{z}_i) \stackrel{\text{iid}}{\sim} \mathbf{U}[0, 1]^d$. This estimator is a sum of squares, hence nonnegative, and it is unbiased. If the true $\tau_u^2 = 0$, then $\hat{\tau}_u^2 = 0$ with probability one. More generally, if the true τ_u^2 is small, then the estimator averages squares of typically small quantities. We assume throughout that $\int f(\mathbf{x})^4 d\mathbf{x} < \infty$ so that the variance of this and our other estimators is finite.

The natural way to estimate τ_u^2 is via

$$\hat{\tau}_u^2 = \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}_i) f(\mathbf{x}_{i,u}:\mathbf{y}_{i,-u}) - \hat{\mu}^2. \quad (5)$$

The simplest estimator of $\hat{\mu}$ is $(1/n) \sum_{i=1}^n f(\mathbf{x}_i)$ but Janon et al. (2012) have recently proved that it is better to use $\hat{\mu} = (1/2n) \sum_{i=1}^n (f(\mathbf{x}_i) + f(\mathbf{x}_{i,u}:\mathbf{y}_{i,-u}))$.

3 The estimators

The problem with (5) is that it has very large variance when $\tau_u^2 \ll \mu^2$. Although τ_u^2 is invariant with respect to shifts replacing $f(\mathbf{x})$ by $f(\mathbf{x}) - c$ for a constant c , the variance of (5) can be strongly affected by such shifts. Sobol' (1990, 1993) recommends shifting f by an amount close to μ , which while not necessarily optimal, should be reasonable.

An approximation to μ can be obtained by Monte Carlo or quasi-Monte Carlo simulation prior to estimation of τ_u^2 . In our simulations we suppose that an oracle has supplied μ and then we compare estimators that do and do not benefit from the oracle.

Another estimator of τ_u^2 was considered independently by Saltelli (2002) and the Masters thesis of Mauntz (2002) under the supervision of S. S. Kucherenko and C. Pantelides. This estimator, called correlated sampling by Sobol' and Myshetskaya (2007) replaces $f(\mathbf{x}_{i,u}:\mathbf{y}_{i,u})$ by $f(\mathbf{x}_{i,u}:\mathbf{y}_{i,u}) - f(\mathbf{y})$ in (5) and then it is no longer necessary to subtract $\hat{\mu}^2$. Indeed the method can be viewed as subtracting the estimate $n^{-2} \sum_{i=1}^n \sum_{i'=1}^n f(\mathbf{x}_i) f(\mathbf{y}_{i'})$ from the sample mean of $f(\mathbf{x}) f(\mathbf{x}_u:\mathbf{y}_{-u})$. That estimator is called "Correlation 1" below.

Sobol' and Myshetskaya (2007) find that even the correlated sampling method has increased variance when μ is large. They propose another estimator replacing the first $f(\mathbf{x}_i)$ by $f(\mathbf{x}_i) - c$ for a constant c near μ . Supposing that an oracle has supplied $c = \mu$ we call the resulting method "Oracle 1" because it makes use of the true μ one time. One could also make use of the oracle's μ in both the left and right members of the cross moment pair. We call this estimator "Oracle 2" below. The fourth method to compare is a new estimator, called "Correlation 2", that uses two random offsets. Instead of replacing $f(\mathbf{x}_i)$ by

Name	Expectation	Cost
Original (5)	$\mu^2 + \mathcal{I}_u^2$	2
Correlation 1	\mathcal{I}_u^2	3
Correlation 2	\mathcal{I}_u^2	4
Oracle 1	\mathcal{I}_u^2	3
Oracle 2	\mathcal{I}_u^2	2

Table 1: Estimators of \mathcal{I}_u^2 with expected value and number of function values required per sample.

$f(\mathbf{x}_i) - \mu$ it draws a third variable $\mathbf{z} \sim \mathbf{U}[0, 1]^d$ and is based on the identity

$$\begin{aligned} & \iiint (f(\mathbf{x}) - f(\mathbf{z}_u : \mathbf{x}_{-u})) (f(\mathbf{x}_u : \mathbf{y}_{-u}) - f(\mathbf{y})) \, d\mathbf{x} \, d\mathbf{y} \, d\mathbf{z} \\ &= (\mu^2 + \mathcal{I}_u^2) - \mu^2 - \mu^2 + \mu^2 - \mathcal{I}_u^2. \end{aligned} \quad (6)$$

We compare the following estimators

$$\frac{1}{n} \sum_{i=1}^n f(\mathbf{x}_i) (f(\mathbf{x}_{i,u} : \mathbf{y}_{i,-u}) - f(\mathbf{y})) \quad (\text{Correlation 1})$$

$$\frac{1}{n} \sum_{i=1}^n (f(\mathbf{x}_i) - f(\mathbf{z}_{i,u} : \mathbf{x}_{i,-u})) (f(\mathbf{x}_{i,u} : \mathbf{y}_{i,-u}) - f(\mathbf{y})) \quad (\text{Correlation 2})$$

$$\frac{1}{n} \sum_{i=1}^n (f(\mathbf{x}_i) - \mu) (f(\mathbf{x}_{i,u} : \mathbf{y}_{i,-u}) - f(\mathbf{y})) \quad (\text{Oracle 1})$$

$$\frac{1}{n} \sum_{i=1}^n (f(\mathbf{x}_i) - \mu) (f(\mathbf{x}_{i,u} : \mathbf{y}_{i,-u}) - \mu) \quad (\text{Oracle 2})$$

where $(\mathbf{x}_i, \mathbf{y}_i, \mathbf{z}_i) \stackrel{\text{iid}}{\sim} \mathbf{U}[0, 1]^{3d}$ for $i = 1, \dots, n$. Not all components of these vectors are necessary to estimate \mathcal{I}_u^2 for a single u , but many applications seek \mathcal{I}_u^2 for several sets u at once, so it is simpler to write them this way. Also, the cost is assumed to be largely in evaluating f , not in producing the inputs $(\mathbf{x}_i, \mathbf{y}_i, \mathbf{z}_i)$. The properties of these estimators are given in Table 1.

The intuitive reason why “Correlation 2” should be effective on small indices is as follows. If the variables in the set u are really unimportant then $f(\mathbf{x})$ will be determined almost entirely by the values in \mathbf{x}_{-u} . Then both $f(\mathbf{x}_i) - f(\mathbf{z}_{i,u} : \mathbf{x}_{i,-u})$ and $f(\mathbf{x}_{i,u} : \mathbf{y}_{i,-u}) - f(\mathbf{y})$ should be small values, even smaller than by centering at μ , and so the estimator takes a mean product of small quantities.

We do not compare the original estimator (5). The bias correction makes it more complicated to describe the accuracy of this method. Also that estimator had extremely bad performance in Sobol’ and Myshetskaya (2007).

Set u	$\underline{\tau}_u^2/\sigma^2$	Corr 1	Corr 2	Orcl 1	Orcl 2
$\{1\}$	0.048	1	4256	518	74
$\{2\}$	0.190	1	1065	525	297
$\{3\}$	0.762	1	267	556	1329
$\{1, 2\}$	0.238	1	774	503	364
$\{1, 3\}$	0.809	1	243	529	1306
$\{2, 3\}$	0.952	1	194	473	1261

Table 2: Relative efficiencies of 4 estimators of $\underline{\tau}_u^2$ for the g -function, rounded to the nearest integer. Relative indices $\underline{\tau}_u^2/\sigma^2$ rounded to three places.

4 Examples

4.1 g function

This is the example used by Sobol’ and Myshetskaya (2007). It has $d = 3$ and

$$f(\mathbf{x}) = \prod_{j=1}^3 \frac{|4x_j - 2| + 2 + 3a}{1 + a_j}.$$

This function has $\mu = 27$ and $\sigma_{\{1\}}^2 = 0.0675$, $\sigma_{\{2\}}^2 = 0.27$, $\sigma_{\{3\}}^2 = 1.08$, $\sigma_{\{1,2\}}^2 = 0.000025$, $\sigma_{\{1,3\}}^2 = 0.0001$, $\sigma_{\{2,3\}}^2 = 0.0004$, $\sigma_{\{1,2,3\}}^2 = 3.7 \times 10^{-8}$. The smallest and therefore probably the most difficult $\underline{\tau}_u^2$ to estimate is $\underline{\tau}_{\{1\}}^2 = \sigma_{\{1\}}^2$. That is the one that they measure.

They report numerical values of $\hat{\underline{\tau}}_{\{1\}}^2/\underline{\tau}_{\{1\}}^2$ for the four estimates in Table 1 (exclusive of the new “Correlation 2” estimate) based on $n = 256,000$ samples. The original estimator gave a values 2.239 times as large as the true $\underline{\tau}_{\{1\}}^2$. The others were ranged from 0.975 to 1.104 times the true value. They did not use the oracle for μ , but centered their estimator instead on $c = 26.8$ to investigate a somewhat imperfect oracle.

The four estimators we consider here are all simply sample averages. As a result we can measure their efficiency by just estimating their variances. The efficiencies of these methods, using “Correlation 1” as the baseline are given by

$$E_{\text{corr 2}} = \frac{3 \text{Var}(\text{corr 1})}{4 \text{Var}(\text{corr 2})}, \quad E_{\text{orcl 1}} = \frac{\text{Var}(\text{corr 1})}{\text{Var}(\text{orcl 1})}, \quad \text{and} \quad E_{\text{orcl 2}} = \frac{3 \text{Var}(\text{corr 1})}{2 \text{Var}(\text{orcl 2})}$$

where the multiplicative factors accounts for the unequal numbers of function calls required by the methods.

The efficiencies of the four estimators are compared in Table 2 based on $n = 1,000,000$ function evaluations. This is far more than one would ordinarily use to estimate the indices themselves, but we are interested in their sampling variances here. We consider all sets except $u = \{1, 2, 3\}$ because $\underline{\tau}_{\{1,2,3\}}^2 = \sigma^2$ which can be estimated more directly. The table contains one small index $\underline{\tau}_{\{1\}}^2$,

Set u	$\underline{\tau}_u^2/\sigma^2$	Corr 1	Corr 2	Orcl 1	Orcl 2
$\{1\}$	0.165	1	0.74	1.13	1.23
$\{2\}$	0.165	1	0.73	1.14	1.24
$\{3\}$	0.041	1	1.69	1.15	0.54
$\{4\}$	0.041	1	1.67	1.15	0.54
$\{5\}$	0.010	1	5.45	1.16	0.20
$\{6\}$	0.010	1	5.58	1.16	0.20
$\{1, 2\}$	0.826	1	0.75	1.21	1.86
$\{3, 4\}$	0.176	1	1.23	1.16	0.94
$\{5, 6\}$	0.042	1	2.94	1.16	0.38

Table 3: Relative efficiencies of 4 estimators of $\underline{\tau}_u^2$ for the product function (7). Relative indices $\underline{\tau}_u^2/\sigma^2$ rounded to three places.

(the one Sobol’ and Myshetskaya (2007) studied). On the small effect, the new Correlation 2 estimator is by far the most efficient, outperforming both oracles. Inspecting the table, it is clear that it pays to use subtraction in both left and right sides of the estimator and that the smaller the effect $\underline{\tau}_u^2$ is, the better it is to replace the oracle’s μ with a correlation based estimate.

4.2 Other product functions

It is convenient to work with functions of the form

$$f(\mathbf{x}) = \prod_{j=1}^d (\mu_j + \tau_j g_j(x_j)) \quad (7)$$

where $\int_0^1 g(x) dx = 0$, $\int_0^1 g(x)^2 dx = 1$, and $\int_0^1 g(x)^4 dx < \infty$. For this function $\sigma_u^2 = \prod_{j \in u} \tau_j^2 \prod_{j \notin u} \mu_j^2$. Taking $g(x) = \sqrt{12}(x - 1/2)$, $d = 6$, $\mu = (1, 1, 1, 1, 1, 1)$ and $\tau = (4, 4, 2, 2, 1, 1)/4$ and sampling $n = 1,000,000$ times lead to the results in Table 3. The results are not as dramatic as for the g -function, but they show the same trends. The smaller $\underline{\tau}_u^2$ is, the more improvement comes from the new estimator. On the smallest indices it beats both oracles.

The improvements for the g -function are much larger than for the product studied here. For the purposes of Monte Carlo sampling the absolute value cusp in the g -function makes no difference. The g -function has the same moments as the product function with $\mu_j = 3$ and $\tau_j = 1/(\sqrt{3}a_j)$. Computing the g function estimates with the product function code (as a check) yields the same magnitude of improvement seen in Table 2.

5 Some generalizations and a recommendation

The best unbiased estimator of $\underline{\tau}_u^2$ is the one that minimizes the variance after making an adjustment for the number of function calls. Unfortunately variances

of estimated variances involve fourth moments which are harder to ascertain than the second moments underlying the ANOVA decomposition.

5.1 More general centering

The estimators in Section 4 are all formed by taking pairs $f(\mathbf{x})$ and $f(\mathbf{x}_u:\mathbf{y}_{-u})$, subtracting centers from them, and averaging the product of those two centered values. Where they differ is in how they are centered.

We can generalize this approach to a spectrum of centering methods.

Theorem 1. *Let v and v' be two subsets of u^c and let $\mathbf{x}, \mathbf{y}, \mathbf{w}, \mathbf{z}$ be independent $\mathbf{U}[0, 1]^d$ random vectors. Then*

$$\mathbb{E}\left((f(\mathbf{x}) - f(\mathbf{x}_v:\mathbf{z}_{-v}))(f(\mathbf{x}_u:\mathbf{y}_{-u}) - f(\mathbf{y}_{v'}:\mathbf{w}_{-v'}))\right) = \underline{\tau}_u^2. \quad (8)$$

Proof.

$$\begin{aligned} & \mathbb{E}\left((f(\mathbf{x}) - f(\mathbf{x}_v:\mathbf{z}_{-v}))(f(\mathbf{x}_u:\mathbf{y}_{-u}) - f(\mathbf{y}_{v'}:\mathbf{w}_{-v'}))\right) \\ &= (\mu^2 + \underline{\tau}_u^2) - (\mu^2 + \underline{\tau}_{\emptyset}^2) - (\mu^2 + \underline{\tau}_{u \cap v}^2) + (\mu^2 + \underline{\tau}_{\emptyset}^2) \\ &= \underline{\tau}_u^2, \end{aligned}$$

because $u \cap v = \emptyset$ and $\underline{\tau}_{\emptyset}^2 = 0$. □

As a result of Theorem 1, we may estimate $\underline{\tau}_u^2$ by

$$\frac{1}{n} \sum_{i=1}^n (f(\mathbf{x}_i) - f(\mathbf{x}_{i,v}:\mathbf{z}_{i,-v}))(f(\mathbf{x}_{i,u}:\mathbf{y}_{i,-u}) - f(\mathbf{y}_{i,v'}:\mathbf{w}_{i,-v'})) \quad (9)$$

where $(\mathbf{x}_i, \mathbf{y}_i, \mathbf{w}_i, \mathbf{z}_i) \stackrel{\text{iid}}{\sim} \mathbf{U}(0, 1)^{4d}$.

The new estimate (9) uses up four independent vectors, not the three used in the Correlation 2 estimator, so we should check that it really is a generalization.

First, suppose that $v' = u^c$. Then the only part of the vector \mathbf{w} that is used in (9) is $\mathbf{w}_{-v'} = \mathbf{w}_u$. Because (9) does not use \mathbf{y}_u the needed parts of \mathbf{y} and \mathbf{w} fit within the same vector. That is we can sample \mathbf{y} as before and use \mathbf{y}_u for \mathbf{w}_u . As a result when $v' = u^c$ we only need three vectors as follows:

$$\frac{1}{n} \sum_{i=1}^n (f(\mathbf{x}_i) - f(\mathbf{x}_{i,v}:\mathbf{z}_{i,-v}))(f(\mathbf{x}_{i,u}:\mathbf{y}_{i,-u}) - f(\mathbf{y}_i)). \quad (10)$$

If we take $v = u^c$ too, then (10) reduces to the Correlation 2 estimator.

At first, it might appear that the Oracle 2 estimator arises by taking $v = v' = \emptyset$, but this is not what happens, even when $\mu = 0$. A more appropriate generalization of the oracle estimators is to based on the identity

$$\underline{\tau}_v^2 = \mathbb{E}((f(\mathbf{x}) - \mu_v(\mathbf{x}_v))(f(\mathbf{x}_u:\mathbf{z}_{-u}) - \mu_{v'}(\mathbf{z}_{v'})))$$

where $\mu_v(\mathbf{x}_v) = \mathbb{E}(f(\mathbf{x}) \mid \mathbf{x}_v)$ and $v, v' \subseteq u^c$. To turn this identity into a practical estimator requires estimation of these conditional expectations. For $v = v' = \emptyset$ the conditional expectations become the unconditional expectation, which is simply the integral of f . For other v and v' , such estimation requires something like nonparametric regression, with bias and variance expressions that complicate the analysis of the resulting estimate.

5.2 Recommendation

The Correlation 2 estimator has $v = v' = u^c$, so it holds constant all of the variables in \mathbf{x}_{-u} . From Theorem 1, we see that this is just one choice among many and it raises the question of which variables should be held fixed in a Monte Carlo estimate of $\hat{\tau}_u^2$. The result is that we find taking $v = v' = u^c$ to be a principled choice.

We can get some insight by considering functions of product form. Even there the resulting variance formulas become cumbersome, but simplified versions yield some insight. We can write it as

$$f(\mathbf{x}) = \prod_{j=1}^d h_j(x_j) \quad (11)$$

where $h_j(x) = \mu_j + \tau_j g_j(x)$ with $\int_0^1 g_j(x)^p dx$ taking values 0, 1, γ_j and κ_j for $p = 1, 2, 3$, and 4 respectively. In statistical terms, the random variable $h_j(x)$ has skewness γ_j/τ_j^3 and kurtosis $\kappa_j/\tau_j^4 - 3$ if $x \sim \mathbf{U}[0, 1]$ and $\tau_j > 0$. We will suppose that all $\tau_j \geq 0$ and that all $\kappa_j < \infty$.

Proposition 1. *Let $\hat{\tau}_u^2$ be given by (9), where f is given by the product model (11). Then, for $v, v' \subseteq u^c$,*

$$n\text{Var}(\hat{\tau}_u^2) = \mathbb{E}(Q_v(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w})Q_{uv'}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w})) - \hat{\tau}_u^4$$

for $\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w} \stackrel{\text{iid}}{\sim} \mathbf{U}[0, 1]^d$ where

$$\begin{aligned} Q_v &= \prod_{j=1}^d h_j^2(x_j) + \prod_{j \in v} h_j^2(x_j) \prod_{j \notin v} h_j^2(z_j) - 2 \prod_{j \in v} h_j^2(x_j) \prod_{j \notin v} h_j(x_j)h_j(z_j), \quad \text{and} \\ Q_{uv'} &= \prod_{j \in u} h_j^2(x_j) \prod_{j \notin u} h_j^2(y_j) + \prod_{j \in v'} h_j^2(y_j) \prod_{j \notin v'} h_j^2(w_j) \\ &\quad - 2 \prod_{j \in u^c \cap v'} h_j^2(y_j) \prod_{j \in u \cap v'^c} h_j(x_j)h_j(w_j) \prod_{j \in u^c \cap v'^c} h_j(y_j)h_j(w_j) \end{aligned}$$

Proof. We need the expected square of the quantity inside the expectation in equation (8). First we expand

$$f(\mathbf{x}) - f(\mathbf{x}_v : \mathbf{z}_{-v}) = \prod_{j=1}^d h_j(x_j) - \prod_{j \in v} h_j(x_j) \prod_{j \notin v} h_j(z_j).$$

Squaring this term yields Q_v , and similarly, squaring

$$f(\mathbf{x}_u: \mathbf{y}_{-u}) - f(\mathbf{y}_{v'}: \mathbf{w}_{-v'}) = \prod_{j \in u} h_j(x_j) \prod_{j \notin u} h_j(y_j) - \prod_{j \in v'} h_j(y_j) \prod_{j \notin v'} h_j(w_j)$$

yields $Q_{uv'}$, after using $u \cap v' = \emptyset$. \square

Using Proposition 1 we can see what makes for a good estimator in the product function setting. The quantities Q_v and $Q_{uv'}$ should both have small variance and their correlation should be small. The latter effect is very complicated depending on the interplay among u , v and v' , and one might expect it to be of lesser importance. So we look at $\mathbb{E}(Q_v^2)$ for insight as to which indices should be in v . Then we suppose that it will usually be best to take the same indices for both v and v' .

Theorem 2. *Let $\hat{\mathcal{L}}_u^2$ be given by (9), where f is given by the product model (11) and let Q_v be as defined in Proposition (1). Then Q_v is minimized over $v \subseteq u^c$ by taking $v = u^c$.*

Proof. Let $\mu_{4j} = \int_0^1 h_j(x)^4 dx$ and $\mu_{2j} = \int_0^1 h_j(x)^2 dx$. It is elementary that $\mu_{4j} \geq \mu_{2j}^2$. Expanding $\mathbb{E}(Q_u^2)$ and gathering terms yields,

$$\begin{aligned} & \prod_{j=1}^d \mu_{4j} + \prod_{j=1}^d \mu_{4j} + 4 \prod_{j \in v} \mu_{4j} \prod_{j \notin v} \mu_{2j}^2 + 2 \prod_{j \in v} \mu_{4j} \prod_{j \notin v} \mu_{2j}^2 \\ & - 4 \prod_{j \in v} \mu_{4j} \prod_{j \notin v} \mu_{2j}^2 - 4 \prod_{j \in v} \mu_{4j} \prod_{j \notin v} \mu_{2j}^2 \\ & = 2 \prod_{j=1}^d \mu_{4j} - 2 \prod_{j \in v} \mu_{4j} \prod_{j \notin v} \mu_{2j}^2. \end{aligned}$$

We minimize this expression by taking the largest possible set $v \subseteq u^c$, that is $v = u^c$. \square

From Theorem 2, we see that the Correlation 2 estimator minimizes $\mathbb{E}(Q_u^2)$ for product functions among estimators of the form (9).

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